

Interface dynamics equations: thier properties and computer simulation.

V.Gafiychuk, A.Shnyr, B.Dacko

Institute of Applied Problems of Mechanics and Mathematics,

National Academy of Science of Ukraine

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Abstract

We investigate the interface dynamic in Laplacian growth model, using the conformal mapping technique. Starting from the governing equation for the conformal map, obtained by B.Shraiman and D.Bensimon, we derive different possible forms of the equation. Some of them have evident physical representation and are convenient for computer simulation, the results of which are presented in this paper.

Formation and evolution of interfaces in systems with phase transition of the first kind led to one of the most striking phenomena of self-organization – the growth of dendritic structures. These phenomena are inherent to many branches of physics, chemistry and biology and are quite similar from mathematical point of view. They are known as the moving boundary problems or Stefan problems [1,2].

Such problems, as usual, have no analytical solutions caused by the essential non-linearity stipulated by the representation of the boundary conditions for parameters, allocated in space on the free boundary. In the given class of systems with free boundaries it is possible to single out a subclass where the distribution of the field in the space is stationary. It is known as quasistationary Stefan problem. Usage of the methods of conformal mapping allows to reduce the last problem to a dynamics of some physical fields in the system with fixed boundaries. This approach is more suitable for analytical and computer simulation.

Theoretical methods of the functions with the complex variable appear to be rather useful in the construction of the effective surface dynamics of the interface at least in the two-dimensional problem. In this case the central part belongs to the conformal mappings of the physical regions of the space onto some special kind of regions. A large number of models for interfacial dynamics have been proposed by now. Reviews of these problems can be found in [3–5]. The most famous equation has been introduced by Shraiman and Bensimon [6] and now is widely known as the conformal mapping equation and it is still under investigation.

Let us consider the problem of Laplacian growth, which can be formulated in the following way. We investigate the growth of two-dimensional region D and suppose, that its boundary ∂D , which represents the physical interface, is the analytic Jordan curve Γ [1]. The field φ outside of the region D , obeys the Laplace equation

$$\Delta\varphi = 0. \tag{1}$$

The boundary ∂D grows at a rate, that is proportional to the normal gradient of the field of the interface. Therefore the evolution of the interface is governed by the following equation

$$v_n = -\nabla_{\mathbf{n}}\varphi|_{\Gamma}. \tag{2}$$

The potential field φ satisfies the following boundary condition at the interface

$$\varphi|_{\Gamma} = d_0 k|_{\Gamma}, \tag{3}$$

where k is the curvature of the interface Γ , d_0 – is the dimensionless surface tension parameter.

FIGURES

FIG. 1. Time-dependent conformal mapping from the exterior of the unit disc onto the domain of our interest.

Equations (1)-(3) determine the boundary-value problem with moving interface, or Stefan problem. Usage of the the methods of conformal mapping [4–12,14], which are based on the Riemann mapping theorem, allows to simplify the considered task. The theorem states the existence of a conformal map from the exterior of D onto a standard domain, for example, the exterior of the unit disk, and boundary ∂D corresponds to unit circle. In outline one can parametrize the evolution of the interface in z plane by the time-dependent conformal map $F(w, t)$, which takes the exterior of the unit disk at each instant of time, $|w| = 1$, onto the exterior of D . Therefore the evolution of the interface can be represented in the terms of

$$\Gamma(\theta, t) = \lim_{w \rightarrow e^{i\theta}} F(w, t), \quad 0 \leq \theta < 2\pi \quad (4)$$

As it is shown by Shraiman and Bensimon [6], in case of free surface tension ($d_0 = 0$) the conformal map fulfills the following equation of motion

$$\frac{\partial \Gamma(\theta, t)}{\partial t} = -i \frac{\partial \Gamma(\theta, t)}{\partial \theta} S \left[\left| \frac{\partial \Gamma(\theta, t)}{\partial \theta} \right|^{-2} \right] \Big|_{w=e^{i\theta}}, \quad (5)$$

where $S[\cdot]$ stands for Schwartz operator. For the exterior of the unit circle with some boundary condition $f(\theta)$ the Schwartz operator can be represented in the following way

$$S[f(\theta)] = -\frac{1}{2\pi} \int_0^{2\pi} d\theta' \frac{e^{i\theta'} + w}{e^{i\theta'} - w} f(\theta') + iC, \quad (6)$$

where C is an arbitrary constant. Denoting the action of the Schwartz operator on $\left| \frac{\partial \Gamma(\theta, t)}{\partial \theta} \right|^{-2}$ as the limit of an analytic function $G(w, t)$, which explicit form is unique and explicitly determinable [7], the equation of motion for $F(w, t)$ (5) is transformed to

$$\frac{dF(w, t)}{dt} = w \frac{dF(w, t)}{dw} G(w, t). \quad (7)$$

Let us also write down the logarithmic derivative of the (7) with respect to w

$$\frac{d}{dt} \ln \frac{dF(w, t)}{dw} = \left(\frac{dF(w, t)}{dw} \right)^{-1} \frac{d}{dw} \left(w \frac{dF(w, t)}{dw} G(w, t) \right). \quad (8)$$

Using the explicit forms of the conformal map $F(w, t)$ one can reduce the partial differential equation (5), governing the interface dynamics, to a set of ordinary differential equations for the dynamics of the critical points of the conformal map [6]. This facilitates the analytical and numerical investigations of the complex behavior in the evolution of the interface [7–9].

In spite of this fact sometimes it is convenient to introduce the following field [5,11,12] for these investigations

$$\eta(\theta, t) = \left| \frac{dF(w, t)}{dw} \right|_{w=e^{i\theta}}^{-1}, \quad (9)$$

which has clear representation – the stretch of the interface $\Gamma(\theta, t)$ under conformal map $F^{-1}(z, t)$. The conformality of $F(w, t)$ demands that the critical points of the map, zeroes of its derivative, all lie within the unit disk. Therefore $\ln \frac{dF(w, t)}{dw}$ is an analytic function outside of the region D . Regarding that

$$\ln \left[\frac{dF(w, t)}{dw} \right] \Big|_{w=e^{i\theta}} = \ln \left| \frac{dF(w, t)}{dw} \right| \Big|_{w=e^{i\theta}} + i \psi(w, t) \Big|_{w=e^{i\theta}}, \quad (10)$$

and solving Schwartz problem outside the unit disc in w plane, one can recover the equation of motion for $F(w, t)$ from the equation of motion for $\eta(\theta, t)$, as well as from $\psi(\theta, t)$ one ($\psi(\theta, t)$ represents oriented angle between tangent vectors τ_w and $\tau_{F(w)} 1$). To keep clear the sense of using (6) we should also write down the relations between $\eta(\theta, t)$ and $\psi(\theta, t)$ [5,12]

$$\psi(\theta, t) = -\frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \ln \eta(\theta', t). \quad (11)$$

In the present paper we investigate the properties of the equation of motion, obtained by Shraiman and Bensimon (5), and derive the equation of motion for $\eta(\theta, t)$, that is more suitable for numerical simulation. In this case let us note that

$$\left| \frac{\partial \Gamma(\theta, t)}{\partial \theta} \right|^{-2} = \left| \frac{dF(w, t)}{dw} \frac{dw}{d\theta} \right|_{w=e^{i\theta}}^{-2} = \left| \frac{dF(w, t)}{dw} \right|_{w=e^{i\theta}}^{-2} = \eta^2(\theta, t), \quad (12)$$

thus $G(w, t) = S(\eta^2(\theta, t))$, where all constants in Schwartz operator are explicitly determinable [5,7]. Regarding the real part of the left side of the equation (8) as $\frac{d}{dt} \ln \left| \frac{dF(w, t)}{dw} \right|$ and simplifying the right side of the equation one can get

$$\frac{d}{dt} \ln \left| \frac{dF(w, t)}{dw} \right| = \operatorname{Re} \left[G(w, t) + w \frac{dG(w, t)}{dw} + wG(w, t) \frac{d}{dw} \ln \frac{dF(w, t)}{dw} \right]. \quad (13)$$

Determining the real part for each term within square brackets of the right side of (13) for $w = e^{i\theta}$

$$\operatorname{Re} [G(w, t)]|_{w=e^{i\theta}} = \eta^2(\theta, t), \quad (14)$$

$$\operatorname{Re} \left[w \frac{dG(w, t)}{dw} \right] \Big|_{w=e^{i\theta}} = \frac{\partial}{\partial \theta} \operatorname{Im} [G(w, t)]|_{w=e^{i\theta}}, \quad (15)$$

$$\begin{aligned} & \operatorname{Re} \left[wG(w, t) \frac{d}{dw} \ln \frac{dF(w, t)}{dw} \right] \Big|_{w=e^{i\theta}} \\ &= \operatorname{Re} \left[wG(w, t) \frac{d}{dw} \left(\ln \left| \frac{dF(w, t)}{dw} \right| + i\psi(w, t) \right) \right] \Big|_{w=e^{i\theta}} = \\ &= -\eta^2(\theta, t) \frac{\partial \psi(\theta, t)}{\partial \theta} + \operatorname{Im} [G(w, t)] \frac{d}{d\theta} \ln \left| \frac{dF(w, t)}{dw} \right| \Big|_{w=e^{i\theta}}, \end{aligned} \quad (16)$$

and taking into account (9), (12) we rewrite the equation (13) in the following form

$$\begin{aligned} \frac{d}{dt} \ln \eta^{-1}(\theta, t) &= \eta^2(\theta, t) + \frac{\partial}{\partial \theta} \operatorname{Im} [G(w, t)]|_{w=e^{i\theta}} - \eta^2(\theta, t) \frac{\partial \psi(\theta, t)}{\partial \theta} \\ &+ \operatorname{Im} [G(w, t)]|_{w=e^{i\theta}} \frac{d}{d\theta} \ln \eta^{-1}(\theta, t). \end{aligned} \quad (17)$$

Taking into account (11) and the fact, that imaginary part of Schwartz problem solution (6) can be written in the terms of

$$\operatorname{Im} [G(w, t)]|_{w=e^{i\theta}} = \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t), \quad (18)$$

one can simplify equation (17) and obtain the following equation of motion for $\eta(\theta, t)$

$$\begin{aligned} \frac{\partial \eta(\theta, t)}{\partial t} &= -\eta^3(\theta, t) - \eta(\theta, t) \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t) + \\ &+ \eta^3(\theta, t) \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \ln \eta(\theta', t) + \\ &+ \frac{\partial \eta(\theta, t)}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t). \end{aligned} \quad (19)$$

The last equation has similar form to the derived one, using the variational principles of conformal maps [5,11,12].

In order to derive the proper equation of motion for $\eta(\theta, t)$ in the presence of surface tension ($d_0 \neq 0$) we should notice, that all we need is to obtain the proper form of $G(w, t)$ for the nonzero surface tension [10].

Thus, one can rewrite the desired evolution equation for mapping (7) in the following form:

$$\frac{dF(w, t)}{dt} = -w \frac{dF(w, t)}{dw} G_0(w, t), \quad (20)$$

where $G_0(w, t)$ is an analytic function of w , which real part on $|w| = 1$ is specified as follows [10]:

$$\text{Re}[G_0(w, t)]|_{w=e^{i\theta}} = \left[\frac{1 - d_0 \text{Re} w \frac{dS[k(w, t)]}{dw}}{\left| w \frac{dF(w, t)}{dw} \right|^2} \right]_{w=e^{i\theta}}. \quad (21)$$

Comparing equations (20) and (7) we should notice, that to derive the equation of motion for the properly introduced $\eta(\theta, t)$, we have to define the real and imaginary parts of $G_0(w, t)|_{w=e^{i\theta}}$

$$\text{Re}[G_0(w, t)]|_{w=e^{i\theta}} = \eta^2(\theta, t) \left(1 - d_0 \frac{\partial}{\partial \theta} \text{Im}[S[k(w, t)]]|_{w=e^{i\theta}} \right) \quad (22)$$

$$\text{Im}[G_0(w, t)]|_{w=e^{i\theta}} = \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t) \left(1 - d_0 \frac{\partial}{\partial \theta'} \text{Im}[S[k(w, t)]]|_{w=e^{i\theta'}} \right), \quad (23)$$

where

$$\text{Im}[S[k(w, t)]]|_{w=e^{i\theta}} = \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} k(\theta', t). \quad (24)$$

After the similar simplifications for the free-tension case one could obtain the following equation of motion for $\eta(\theta, t)$:

$$\frac{\partial \eta(\theta, t)}{\partial t} = -\eta^3(\theta, t) \left(1 - d_0 \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} k(\theta', t) \right) +$$

$$\begin{aligned}
& -\eta(\theta, t) \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t) \left(1 - d_0 \frac{\partial}{\partial \theta'} \frac{1}{2\pi} \int_0^{2\pi} d\theta'' \coth \frac{\theta'' - \theta'}{2} k(\theta'', t) \right) + \\
& + \eta^3(\theta, t) \left(1 - d_0 \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} k(\theta', t) \right) \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \ln \eta(\theta', t) + \\
& + \frac{\partial \eta(\theta, t)}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \eta^2(\theta', t) \left(1 - d_0 \frac{\partial}{\partial \theta'} \frac{1}{2\pi} \int_0^{2\pi} d\theta'' \coth \frac{\theta'' - \theta'}{2} k(\theta'', t) \right), \quad (25)
\end{aligned}$$

where $k(\theta, t)$ is the curvature of $\Gamma(\theta, t)$:

$$k(\theta, t) = -\eta(\theta, t) \frac{\partial \psi(\theta, t)}{\partial \theta} = \eta(\theta, t) \frac{\partial}{\partial \theta} \frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \ln \eta(\theta', t). \quad (26)$$

One can also notice [5,10,12] that

$$v_n(\theta, t) = \eta(\theta, t) \left(1 - d_0 \frac{\partial}{\partial \theta} \text{Im} [S[k(w, t)]]|_{w=e^{i\theta}} \right) \quad (27)$$

Equations (25)-(27) represent the system of integrodifferential equations that fully describes the evolution of the interface.

To solve the derived singular integral equations with Hilbert kernel, the useful approach is developed, based on interpolation of the expressions of integration in singular integrals by trigonometric polynomial. For example, for each number $N = 2n$ of the nodes we can use the formulae [13]

$$\tilde{f}_n(\theta) = \frac{1}{2\pi} \sum_{j=0}^{2n-1} \tilde{f}(\theta_j) \sin[n(\theta - \theta_j)] \cot \frac{\theta - \theta_j}{2} \quad (28)$$

$$\theta_j = \frac{\pi j}{n}, \quad j = 0, 1, \dots, 2n-1 \quad (29)$$

which lead to the next integral representation:

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta' \coth \frac{\theta' - \theta}{2} \tilde{f}(u_j) = \frac{1}{2n} \sum_{j=0}^{2n-1} \tilde{f}(\theta_j) \cot \frac{\theta_j - \theta_m^0}{2} \quad (30)$$

where

$$u_m^0 = \frac{2\pi m + 1}{2\pi}, \quad m = 0, 1, \dots, 2n-1 \quad (31)$$

The system of nonlinear integrodifferential equations was investigated numerically. The basis of the numeric simulation was the approximation of unknown quantities of functions by above mentioned trigonometrical polynomial. Expansions of this type make it possible to use well-known quadrature formulae to evaluate singular Integrals . As a result, the system of equations (25),(26) and (27) reduces to a system of ordinary non-linear equations with full Jacobian.

It is possible to reproduce geometrically defined interfaces in parametric form by using the equations:

$$\begin{aligned} dy &= \frac{d\theta}{\eta(\theta, t)} \sin \left(\theta + \psi(\theta) + \frac{\pi}{2} \right) \\ dx &= \frac{d\theta}{\eta(\theta, t)} \cos \left(\theta + \psi(\theta) + \frac{\pi}{2} \right) \end{aligned} \quad (32)$$

In numerical experiment the evolution of the form of an interface of phases in an association from an aspect of initial perturbations $\delta\eta|_{t=0}$ of a surface energy d_0 was investigated.

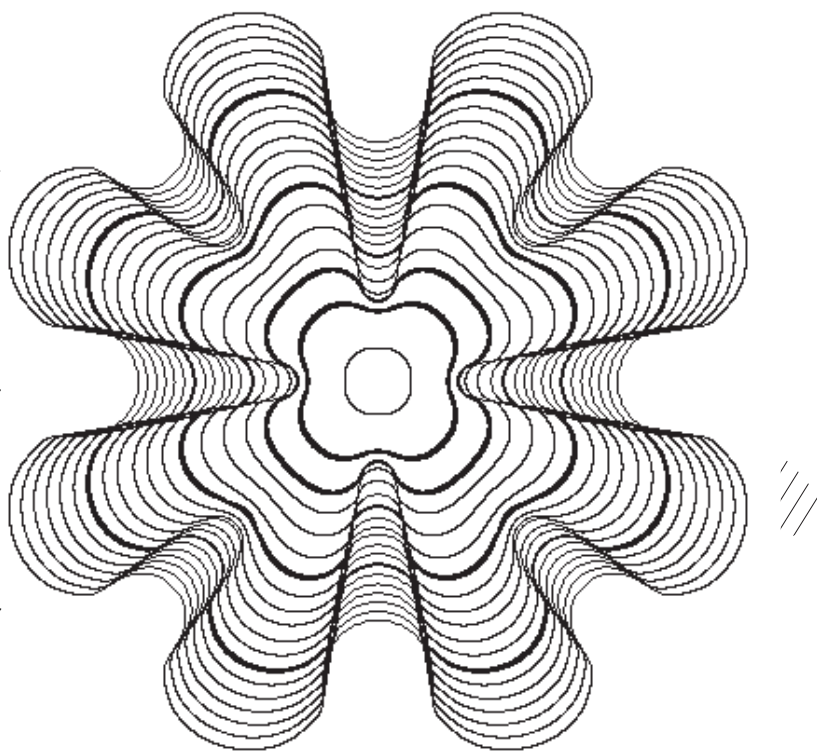
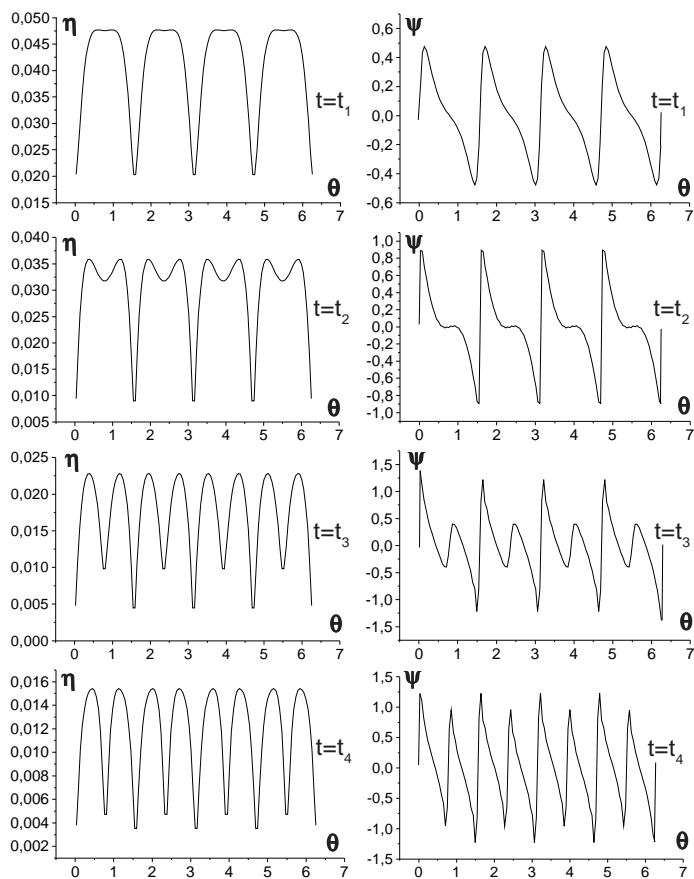
Figures (2) and (3) illustrate the characteristic form of non-uniform distributions of the η , ψ and the corresponding interfaces for different initial perturbations. The reader should observe that relatively smooth variations of the interface correspond to quite marked variations in the field η and hence also in the angle ψ . Thus, relatively small errors in determining do not cause marked changes in the interface geometry. In addition, as is evident from the figures, relatively even long sections of the Interface contract when mapped into the interval $[0, 2\pi]$, whereas pronounced changes in the contour Γ , conversely, are stretched out. In this sense such mappings of onto are "adaptive" with respect to information about the detailed geometric structure of the interface.

FIG. 2. Non-uniform distributions of the $\eta(\theta, t)$, $\psi(\theta, t)$ and the corresponding interfaces for the following initial perturbation: $\eta(\theta, t_0 = 0) = 0.1 - 0.01 \cos(4\theta)$; $d_0 = 0.1$; $t_1 = 500$; $t_2 = 1000$; $t_3 = 3000$; $t_4 = 6000$. Bold interfaces on the figure correspond to mentioned above instances of time.

FIG. 3. Non-uniform distributions of the $\eta(\theta, t)$, $\psi(\theta, t)$ and the corresponding interfaces for the following initial perturbation: $\eta(\theta, t_0 = 0) = 0.1 - 0.01 \cos(6\theta)$; $d_0 = 0.1$; $t_1 = 500$; $t_2 = 1000$; $t_3 = 3000$; $t_4 = 6000$. Bold interfaces on the figure correspond to mentioned above instances of time.

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z -plane

